

Bridging physics-based and data-driven modelling

Introduction

Materials modelling within science and engineering traditionally use physics-based models, but currently there is much excitement about big data and machine learning in materials and molecular modelling, and about the opportunities that these approaches may bring. But are there also scientific shortcomings associated? Is this development in fact driving us towards "... numbers, not insights", i.e. away from the often quoted scientific wish for "... insights, not numbers"?! Can we come to an understanding in the community about how physics-based insight and data-driven analysis may complement each other?

Objectives

The objective of this session is to gather information on

- how European industry perceives the future role of machine learning (ML) and informatics in materials modelling, and
- how to best use ML and informatics (together with physics-based models) to achieve efficient strategies, including C&L, to overcome current model gaps for industrial modelling,
- how to best achieve synergies between physics-based and data-driven modelling (collect feedback on and collect successful and not so successful examples)

Background information and documents

Relevant information for this session can be found in the following documents:

- The Review of Materials Modelling (RoMM) 6, which provides the required vocabulary and classification for models and workflows.
<https://publications.europa.eu/en/publication-detail/-/publication/ec1455c3-d7ca-11e6-ad7c-01aa75ed71a1>

Discussion points and questions

The following questions summarize the issues for this session.

- What are the pros and cons of physics-based and data-driven modelling in industry?
- Which approaches are perceived as the most reliable and trustworthy - and why?
- Are there examples of successful integration of machine learning (ML) with physics-based modelling within different industrial sectors?
- Are there educational examples (successes or failures) of the use of machine learning (ML) within different industrial sectors?
- Will we be able to get deep scientific insights, or even physics theories, from ML?
- Where will we be 5 years from now? 10 years from now?